201-16128

IUCLID

Data Set

Existing Chemical	:	ID: 2611-00-9
CAS No.	:	2611-00-9
EINECS Name	:	cyclohex-3-enylmethyl cyclohex-3-enecarboxylate
EC No.	:	220-031-5
Molecular Formula	:	C14H20O2
Producer related part		
Company	:	The Dow Chemical Company
Creation date	:	01.12.0005
Substance related part		
Company	:	The Dow Chemical Company
Creation date	:	01.12.0005
Status	:	
Memo	:	
Printing date	:	20.12.2005
Revision date	:	
Date of last update	:	20.12.2005
Number of pages	:	27
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1. General Information

Id 2611-00-9
Date 20.12.2005

1.0.1 APPLICANT AND COMPANY INFORMATION

Type	:	manufacturer
Name	:	Dow Chemical
Contact person	:	
Date	:	01.12.2005
Street	:	
Town	:	48674 Midland, MI
Country	:	United States
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

05.12.2005

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

Type	:	manufacturer
Name of plant	:	
Street	:	
Town	:	
Country	:	United States
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

01.12.2005

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name	:	
Smiles Code	:	O=C(OCC(CCC=C1)C1)C(CCC=C2)C2
Molecular formula	:	C14 H20 O2
Molecular weight	:	220.31
Petrol class	:	

09.12.2005

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	typical for marketed substance

Substance type	:	organic
Physical status	:	liquid
Purity	:	
Colour	:	Transparent colorless
Odour	:	Sweet

01.12.2005

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

3-Cyclohexene-1-Carboxylic Acid, 3-Cyclohexen-1-ylmethyl ester

05.12.2005

3-Cyclohexenyl 3-Cyclohexene 1-Carboxylate

05.12.2005

Diene 221

05.12.2005

1.3 IMPURITIES

Purity	:	typical for marketed substance
CAS-No	:	
EC-No	:	
EINECS-Name	:	4-(hydroxymethyl)1-cyclohexene
Molecular formula	:	
Value	:	<= 1 % v/v

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Purity	:	typical for marketed substance
CAS-No	:	100-50-5
EC-No	:	202-858-3
EINECS-Name	:	cyclohex-3-ene-1-carbaldehyde
Molecular formula	:	C7 H10 O1
Value	:	<= .3 % v/v

16.12.2005

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use	:	industrial
Category	:	Chemical industry: used in synthesis
Remark	:	Intermediate closed system
15.12.2005		

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

Source of exposure	:	other: Closed system intermediate - exposure is negligible
Exposure to the	:	

01.12.2005

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= 47 °C
Sublimation	:	
Method	:	other: calculated MPBPVP
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4

19.12.2005 (1)

2.2 BOILING POINT

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= .001746523 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated):MPBPWin
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4

19.12.2005 (2)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	ca. 4.97 at °C
pH value	:	
Method	:	other (calculated):KOWWIN
Year	:	
GLP	:	
Test substance	:	

19.12.2005 (2)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 1.94 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	

Stable	:	
Deg. product	:	
Method	:	other:WSKOWWIN
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4

19.12.2005 (2)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	other:calculated
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
DIRECT PHOTOLYSIS		
Halflife t1/2	:	= .1 day(s)
Degradation	:	% after
Quantum yield	:	
INDIRECT PHOTOLYSIS		
Sensitizer	:	O3
Conc. of sensitizer	:	
Rate constant	:	= cm^3/(molecule*sec)
Degradation	:	% after
Deg. product	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	

Remark : The fact that Diene 221 absorbs light in the >290 nm wavelength range merely indicates that photodecay is possible (aqueous photolysis the most likely pathway). Kent Woodburn, personal communication 2005.

Result : Summary (AOP v1.91)

Reaction with N, S and -OH = 0.0000E-12 cm3/moleculoe-sec
Overall OH Rate Constant = 126.5794 E-12 cm3/moleucle-sec
Half-life = 0.085 Days (12-hr day; 1.5E6 OH/cm3)

Summary (AOPv1/91): Ozone Reaction
Overall Ozone Rate Constant = 40 E-17 cm3/molecule-sec
Half-life = 0.029 Days (at 7E11 mol/cm3)

19.12.2005 (3)

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)

Soil : % (Fugacity Model Level II/III)
Method : other:calculated
Year :

Method : Level III Fugacity Model; July 2004. Level III model version 2.80.1. Obtained from the Canadian Environmental Modeling Centre, Trent University, Peterborough, Ontario, Canada.
Attached document : Diene 221.doc
Conclusion : This substance has a predicted moderate vapor pressure and low water solubility, is readily biodegradable, has a predicted high reactivity in air, and adsorbs readily to soil/sediment surfaces due to its elevated lipophilicity (i.e., high Kow). If released to water, the compound will be fairly evenly distributed between water and sediment and should undergo primary biodegradation rapidly. If released to soil, virtually the entire mass of chemical will remain in soil, where it will also undergo primary biodegradation very rapidly. If released to air, the compound will remain largely in air and undergo rapid degradation through reaction with hydroxyl radicals and ozone. Finally, if released to all three compartments equally, a majority will be associated with soil and the remainder fairly well distributed between water sediment. In each case, the ubiquitous nature of esterases will produce rapid primary biodegradation of the molecule. Personal communication Kent Woodburn 2005.
Reliability : (2) valid with restrictions
(2): Valid with restrictions: Accepted calculation method. Klimish rating. Klimish HJ et al, Regulatory Toxicology and Pharmacology 1997; 25:1-5.

19.12.2005 (4)

METHOD
Test: Predicted transport between environmental compartments
Method: Level III Fugacity Model
Year: July 2004
Remarks: Level III model version 2.80.1. Obtained from the Canadian Environmental Modeling Centre, Trent University, Peterborough, Ontario, Canada [1].

Input Parameters for Level III Model:

Property	Value	Source
Data Temperature (°C)	25	Default environmental temperature
Chemical Type	1	Type 1 indicates chemical can partition into all environmental compartments
Molecular Mass (g/mol)	220.3	Calculated from molecular structure
Water Solubility (g/m^3)	1.94	Calculated via WSKOWWIN [2]
Vapor Pressure @ 25°C (Pa)	0.17	Calculated via MPBPVP [2]
Melting Point (°C)	47	Calculated via MPBPVP [2]
Henry's Law Constant (Pa*m^3/mole)	0.86	Calculated via HENRYWIN [2]
Log K_{ow} (Octanol-Water Partition Coefficient)	4.97	Calculated via KOWWIN [2]
Simulated Emission Rate (kg/hr)	1,000	Level III Default Values [1]
Simulated Environment	Default Level III environment [1]	
Reaction Half-lives (hr) Input to Level III Model:		
Air (vapor phase)	0.41	Estimated half-life in air via AOPWIN [2]
Water (no susp. solids)	3,60*	Estimated half-lives in water, soil, and sediment extrapolated from predicted inherent biodegradability [2].
Soil	7,20*	
Sediment	3,240*	
Suspended Sediment	**1.0 x 10^{11}	
Fish	**1.0 x 10^{11}	
Aerosol	**1.0 x 10^{11}	

*Half-lives extrapolated from predicted inherent biodegradability, according to Technical Guidance Document of the European Commission [3]. **Default value used in Level III model when reaction is expected to be negligible in this compartment.

RESULTS
Level III: Predicted distribution among air, water, soil, and sediments

Emission Scenario	Percentage and amount distributed to				Residence Time (days) [without advection in brackets]
	Air	Water	Soil	Sediment	
1,000 kg/hr to Air	86.6% 583 kg	1.4% 9 kg	10.3% 69 kg	<0.1% 11 kg	<0.1 [<0.1]
1,000 kg/hr to Water	<0.1% 144 kg	45.1% 2.5E5 kg	<0.1% 17 kg	54.9% 3.0E5 kg	23 [30]
1,000 kg/hr to Soil	<0.1% 1.2 kg	<0.1% 191 kg	100.0% 1.0E6 kg	<0.1% 233 kg	43 [43[
1,000 kg/hr simultaneously to Air, Water, and Soil	<0.1% 729 kg	15.6% 2.5E5 kg	65.3% 1.0E6 kg	19% 3.0E5 kg	22 [24]

Highlighted scenario indicates most probable emission route, based on physical properties and use patterns.

3.3.2 DISTRIBUTION

Media :
Method : Calculation according Mackay, Level I
Year :

Method : Prediction of Equilibrium Environmental Distribution
Method: Level I Fugacity Model, Version 3.00
Year: September 2004
Remarks: Level I model version 3.00, Obtained from the Canadian Environmental Modeling Centre, Trent University, Peterborough, Ontario, Canada.

Attached document : Diene 221 Fugacity Level I.doc

Conclusion : This substance has a low predicted water solubility, moderate vapor pressure, and high log Kow.; the substance therefore has a high potential for adsorption to soil or sediments. In the absence of advective and reactive processes, these physical properties dictate that the substance will be largely distributed to the soil compartment at equilibrium.

Reliability : (2) valid with restrictions
(2): Valid with restrictions: Accepted calculation method. Klimish rating. Klimish HJ et al, Regulatory Toxicology and Pharmacology 1997; 25:1-5.

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Property	Value	Source
Data Temperature (°C)	25	Default environmental temperature
Chemical Type	1	Type 1 indicates chemical can partition into all environmental compartments
Molecular Mass (g/mol)	220.3	Calculated from molecular structure
Water Solubility (g/m^3)	1.94	Calculated via WSKOWWIN [2]
Vapor Pressure @ 25°C (Pa)	0.17	Calculated via MPBPVP [2]
Melting Point (°C)	47	Calculated via MPBPVP [2]
Henry's Law Constant ($Pa*m^3/mole$)	0.86	Calculated via HENRYWIN [2]
Log K_{ow} (Octanol-Water Partition Coefficient)	4.97	Calculated via KOWWIN [2]
Simulated Emission (kg)	100,000	Level I Default Value [1]
Simulated Environment	Default Level I environment [1]	

RESULTS

Level I: Predicted equilibrium distribution among air, water, soil, and sediments

Emission Scenario	Percentage and amount distributed to			
	Air	Water	Soil	Sediment
100,000 kg total emissions	0.5 % 532 kg	1.16 % 1163 kg	96.1 % 96098 kg	2.1 % 2135 kg

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Contact time	:	
Degradation	:	(±) % after
Result	:	other
Deg. product	:	
Method	:	other:BIOWin
Year	:	
GLP	:	
Test substance	:	

Remark : Personal communication - Kent Woodburn (2005): Should be readily biodegradable and BIOWIN modeling supports this assumption.

19.12.2005

3.6 BOD5, COD OR BOD5/COD RATIO

BOD5		
Method	:	other:calculated
Year	:	
Concentration	:	related to
BOD5	:	mg/l
GLP	:	
COD		
Method	:	other:calculated
Year	:	
COD	:	mg/g substance
GLP	:	

Remark : Personal communication - Kent Woodburn (2005): Should be readily biodegradable and BIOWIN modeling supports this assumption.

19.12.2005

3.7 BIOACCUMULATION

Elimination	:	
Method	:	other
Year	:	
GLP	:	
Test substance	:	

Remark : Personal communication - Kent Woodburn (2005): While the high estimated log Kow value of approximately 5 indicates a potential for bioaccumulation, the instability of the compound in water/soil/sediment will produce as the major metabolite the carboxylic acid, which is highly water soluble and will not pose a bioaccumulation hazard.

Should undergo metabolism via esterases to the corresponding carboxylic acid.

19.12.2005

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	other:Estimated
Species	:	other:freshwater fish
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	ca. .859 calculated
Method	:	other:ECOSAR
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4

02.12.2005 (6)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	other:estimated
Species	:	Daphnia sp. (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EC50	:	ca. .347 calculated
Method	:	other:ECOSAR
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4

02.12.2005 (6)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	other algae:green alga
Endpoint	:	growth rate
Exposure period	:	96 hour(s)
Unit	:	mg/l
EC50	:	ca. .076 calculated
Method	:	other:ECOSAR
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4

05.12.2005 (6)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 2386 - 1363 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	5
Vehicle	:	other: undiluted
Doses	:	Male: 1000, 2000, 4000 and 8000 mg/kg Female: 1000, 1400 and 2000 mg/kg
Method	:	other:essentially followed OECD guideline 420 fixed doses
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Rats ranging from 200 - 300 grams in weight were used in this study. Five male or female rats per dose level were administered the undiluted test material via stomach intubation. The rats were maintained on appropiate commercial diet and municipal water. Both are available ad libitum except during periods of fasting. Dosage levels for the toxicity test normally doffer by a factor of 2 in a geometric series, but may differ by other constant factors if required. The maximum dosage for the peroral test is 16 ml/kg. Doses are reduced until significant signs of toxicity are not observed. LD50's and the estimated LD50 slopes are calculated by the moving average method (Thompson W, Bact. Rev., 11:115-141 1947; Weil, 1983) and are based on a 14-day observation period. Animal weights are recorded at 0 days (before dose), 7 days and 14 days (just prior to sacrifice). At death or sacrifice, each animal is subjected to gross pathologic evaluation.
Result	:	Signs of toxicity included sluggishness, lacrimation, prostration, kyphosis (in 2), red cruast on perinasal fur and emaciation (in one). Deaths occurred at one to 2 days. Most survivors recovered at one to 5 days. One female recovered at 11 days. Animals that died had pink to red lungs at necropsy. Survivors had no remarkable lesions.
Test substance	:	Clear, colorless non-viscous liquid Percent composition >98%
Conclusion	:	LD50 males = 2386 mg/kg LD50 females = 1363 mg/kg The toxicity terminology used indicated that the LD50 is an extremely low order.
Reliability	:	(1) valid without restriction 1d: Meets generally accepted scientific standards and is described in sufficient detail. Klimish rating. Klimish HJ et al, Regulatory Toxicology and Pharmacology 1997; 25:1-5.

16.12.2005 (7)

Type	:	LD50
Value	:	= 2836 mg/kg bw

Species	:	rat
Strain	:	other: Carworth Farms-Elias
Sex	:	male
Number of animals	:	5
Vehicle	:	other: undiluted
Doses	:	2000, 4000, 8000 mg/kg bw
Method	:	other:essentially followed OECD guideline 420 fixed doses
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4

Method : Five to six week old rats ranging from 90-120 grams in weight were dosed at levels differing by a factor of 2.0 in a geometric series. The rats were reared in the labs own colony and maintained from time of weaning on Rockland rat diet (complete). The method of moving average for calculating the median-effective dose (LD50) was applied to the 14-day mortality data.

Five male rats per dose level were administered the undiluted test material by stomach tube.

Result : All rats at the 8000 mg/kg group died by day 1; 4 rats at the 4000 mg/kg level died by day 2; and 1 rat at the 2000 mg/kg level died by day 1.

Deaths at the highest dose level occurred within four hours after dosing and were preceded by a narcotic-like stae whild other fatalities were delayed from 24 to 48 hours. Autopsy revealed congestion throughout the lungs and the abdominal viscera.

Test substance : Lot identification - 384RD35

16.12.2005 (8)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Value	:	
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	5
Vehicle	:	
Doses	:	
Exposure time	:	6 hour(s)
Method	:	other:essentially followed OECD guideline 403 Acute Inhalation Toxicity
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4

Method : Five rats per sex weighing between 200 and 300 grams were tested. Essentially saturated test material vapor was produced by passing air (at 2.5 liters/min) through the sample and then through a 9-liter animal chamber (dynamic airflow conditions).

The vapor is produced by enclosing the test material in a sealed 120-liter animal chamber by passing air (at 2.5 liters/min) through the sample and then through a 9-liter animal chamber (dynamic conditions). The chamber oxygen content is mainitained at approximately 20%.

The rats were maintained on appropiate commercial diet and municipal water. Both are available ad libitum except during periods of manipulation. Dosage levels for the toxicity test normally doffer by a factor of 2 in a geometric series, but may differ by other constant factors if required.

Doses are reduced until significant signs of toxicity are not observed.

LD50's and the estimated LD50 slopes are calculated by the moving average method (Thompson W, Bact. Rev., 11:115-141 1947; Weil, 1983) and are based on a 14-day observation period.

Result : There were no deaths of male or female rats during or following the 6-hour test. There were no signs of toxicity or unusual gross pathology observations in either sex.

Test substance : Clear, colorless non-viscous liquid
Percent composition >98%

Reliability : (1) valid without restriction
1d: Meets generally accepted scientific standards and is described in sufficient detail. Klimish rating. Klimish HJ et al, Regulatory Toxicology and Pharmacology 1997; 25:1-5.

16.12.2005 (7)

Type : LC50
Value :
Species : rat
Strain : other:CFE
Sex : female
Number of animals : 6
Vehicle :
Doses :
Exposure time : 8 hour(s)
Method : other:method not indicated
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Method : Concentrated vapor was generated at a temperature of 21C by passing dried air at the rate of 2.5 liters/minute through a fritted glass disc immersed to a depth of at least one inch in 50 ml. of Diene-221.

Remark : The amount of test material used during the 8-hour exposure was not documented in the report.
The LC50 calculation that was used was not documented in the report.

Result : There were no deaths in a range-finding acute inhalation test where 6 female rats were exposed to concentrated vapors at 21 degrees C for 8-hours. The rats gained weight at a subnormal rate during the subsequent two-week observation period. At necropsy on the 14th day, two rats had focal consolidation of the lungs.

Test substance : Lot identification - 384RD35

16.12.2005 (8)

Type : LC50
Value :
Species : rat
Strain : no data
Sex : female
Number of animals : 6
Vehicle :
Doses :
Exposure time : 8 hour(s)
Method : other:method not indicated
Year :
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Method : Concentrated vapor was generated at a high temperature by passing dried air at the rate of 2.5 liters/minute through a fritted glass disc which was submerged in a silicone oil bath that was maintained at a temperature sufficiently high to keep the Diene-221 at approximately 170C. The

ambient air temperature in the 9-liter inhalation chamber averaged about 27C. Diene-221 changed from a colorless liquid to a dark caramel-colored material during the process.

Result : A group of six female rats survived an eight-hour exposure to mist, vapors, and decomposition products atmosphere but three were found dead the following morning. Necropsy revealed lung hemorrhage as the principal cause of death.

Test substance : Lot identification - 384RD35

Reliability : (3) invalid
3b; Invalid Significant metholodological deficiencies. Klimish rating.
Klimish HJ et al, Regulatory Toxicology and Pharmacology 1997; 25:1-5.

This study is considered invalid because there was significant degradation of the material due to a color change during heating (The material changed from a colorless liquid to a dark caramel-colored material). It is therefore unclear what the animals were actually exposed to.

16.12.2005 (8)

Type : LC50
Value : ca.
Species : rat
Strain : no data
Sex :
Number of animals : 6
Vehicle :
Doses :
Exposure time : 4 hour(s)
Method : other:method not indicated
Year :
GLP : no
Test substance : as prescribed by 1.1 - 1.4

Method : Concentrated vapor was generated at a high temperature by passing dried air at the rate of 2.5 liters/minute through a fritted glass disc which was submerged in a silicone oil bath that was maintained at a temperature sufficiently high to keep the Diene-221 at approximately 170C. The ambient air temperature in the 9-liter inhalation chamber averaged about 27C. Diene-221 changed from a colorless liquid to a dark caramel-colored material during the process.

Result : A group of 6 rats survived a four-hour inhalation exposure to mist, vapors, and decomposition products atmosphere and gained weight during the subsequent two-week observation period. On necropsy, day 14, two of the six animals had areas of focal lung consolidation.

Test substance : Lot identification - 384RD35

Reliability : (3) invalid
3b; Invalid Significant metholodological deficiencies. Klimish rating.
Klimish HJ et al, Regulatory Toxicology and Pharmacology 1997; 25:1-5.

This study is considered invalid because there was significant degradation of the material due to a color change during heating (The material changed from a colorless liquid to a dark caramel-colored material). It is therefore unclear what the animals were actually exposed to.

16.12.2005 (8)

5.1.3 ACUTE DERMAL TOXICITY

Type : LD50
Value : = 12325 - 13427 mg/kg bw
Species : rabbit
Strain : New Zealand white

Sex	:	male/female
Number of animals	:	5
Vehicle	:	
Doses	:	4000 (female), 8000, 11300 and 16000 mg/kg
Method	:	other:essentially followed OECD guideline 402 Acute Dermal Toxicity
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	New Zealand White rabbits (5/sex except the 4.0 ml/kg level which only had 2 females), weighing between 2.0 and 3.0 kg, were subjected to 24 hours of contact with Diene-221 which was retained under impervious sheeting on the clipped, intact skin of the trunk. As necessary for larger doses, gauze was wrapped around the trunk over the sample to prevent leakage. Vetrap Bandaging Tape was wrapped over the impervious sheeting and the rabbit was returned to its cage for the contact period. Doses are varied by adjusting the volume or weight of the test material. After the contact period, excess fluid was removed to diminish ingestion. Observations for skin reaction were made at one hour, 7 days and 14 days after the contact period.
Result	:	Local dermal effects included erythema, edema, ecchymosis (in one), alopecia (in one) and desquamation. Sluggishness, unsteady gait (in two), diarrhea (in one) and emaciation (in one) were among the signs of toxicity observed. Time to death ranged from 3 to 8 days. Survivors recovered at 2 to 4 days. Gross pathologic findings included pink to red lungs, red tracheas, stomachs with black or white foci, one liver with tan discoloration and red fluid in the thoracic cavity (in two).
Test substance	:	Clear colorless non-viscous liquid TK3651
Conclusion	:	LD50 male rabbits = 12325 mg/kg LD50 female rabbits = 13427 mg/kg
Reliability	:	(1) valid without restriction 1d: Meets generally accepted scientific standards and is described in sufficient detail. Klimish rating. Klimish HJ et al, Regulatory Toxicology and Pharmacology 1997; 25:1-5.

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Type	:	LD50
Value	:	= 5010 mg/kg bw
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	male
Number of animals	:	8
Vehicle	:	other:undiluted
Doses	:	5010 and 10000 mg/kg
Method	:	other:essentially followed OECD guideline 402 Acute Dermal Toxicity
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Eight male albino New Zealand rabbits, three to five months of age and averaging 2.5 kg were immobilized during the 24-hour contact period. The doses were 5,000 and 10,000 mg/kg. Thereafter, the polyethylene sheeting used to retain the dose in contact with the clipped skin of the trunk was removed and the animals were caged for the remainder of the 14-day observation period. The moving average method of calculating the LD50 was used.
Result	:	Deaths occurred from three to six days after application of Diene 221. For the high dose animals 2 died at 3 days; one died at four days; and one died at five days. For the 5000 mg/kg dose group one died at five days and one died at six days. The remaind two live until study termination. Gross necropsy disclosed some lung congestion, dark mottled livers with acini

prominent, and pale mottled kidneys. The urine of two rabbits contained what appeared to be blood.

Test substance : Lot identification - 384RD35

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5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species	:	rabbit
Concentration	:	undiluted
Exposure	:	Occlusive
Exposure time	:	4 hour(s)
Number of animals	:	6
Vehicle	:	other:undiluted
PDII	:	
Result	:	slightly irritating
Classification	:	
Method	:	other:essentially followed OECD 404 Acute Dermal Irritation
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4

Method : Male or female New Zealand white rabbits were dosed with 0.5 ml. The dose was applied to the clipped, intact skin under a gauze patch and was loosely covered with impervious sheeting. Diene-221 was applied to each of 6 rabbits, which were restarined for the 4-hour contact period. Excess sample was removed after contact. Skin reaction was scored, by the Draize method, at one hour, one day, 2 days, 3 days, and 7 days.

Result : Minor erythema 1/6 and minor edema 4/6. After 2 days, no irritation was present. Desquamation appeared on 5/6 after 7 days, but no other reaction was apparent.

Test substance : Clear, colorless non-viscous liquid
Percent composition >98%

Reliability : (1) valid without restriction
1d: Meets generally accepted scientific standards and is described in sufficient detail. Klimish rating. Klimish HJ et al, Regulatory Toxicology and Pharmacology 1997; 25:1-5.

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Species	:	rabbit
Concentration	:	undiluted
Exposure	:	Open
Exposure time	:	no data
Number of animals	:	5
Vehicle	:	other:none
PDII	:	
Result	:	slightly irritating
Classification	:	
Method	:	other:method not indicated
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4

Remark : No information on method

Result : Uncovered application of 0.01 ml amounts of Diene-221 to the clipped skin of the rabbit belly resulted in no reation on four animals and marked capillary injection on a fifth. Grade 2 in a 10 grade rating system.

Test substance	:	Lot identification - 384RD35
Reliability	:	(3) invalid 3b; Invalid Significant metholodological deficiencies. Klimish rating. Klimish HJ et al, Regulatory Toxicology and Pharmacology 1997; 25:1-5. This study is considered invalid because the liquid was applied without a gauze patch to the skin. Access by the animal to the test material was not prevented. Also accoring to the OECD guideline 404 a 0.5 ml of test material should be applied. Only 0.01 ml was applied. It is therefore unclear what the animals were actually exposed to.

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5.2.2 EYE IRRITATION

Species	:	rabbit
Concentration	:	undiluted
Dose	:	.1 ml
Exposure time	:	
Comment	:	no data
Number of animals	:	6
Vehicle	:	none
Result	:	slightly irritating
Classification	:	irritating
Method	:	other:essentially followed OECD 405 Acute Eye Irritation
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	The dose is instilled into the lower conjunctival sac of one eye per animal. The eyelids are held together for one second. Six eyes are dosed per test volume. The eyes are scored at one hour, approximately 4 hours, one day, 2 days, 3 days and 7 days post-dosing. Fluorescein (2%) staining was used to determine corneal injury before dosing and at readings after one day.
Result	:	Instillation of 0.1 ml of test material into rabbit eyes resulted in no corneal injury or iritis in any of the 6 animals. Minor conjuctival irritation developed in 4 rabbits and all eyes exhibited substantial ocular discharge. By 24 hours, 3 eyes had a normal appearance. One eye still had minor conjuctival redness and 2 had slight discharge. All 6 eyes were healed at 48 hours. Observations continued for 7 days after treatment.
Test substance	:	Clear, colorless non-viscous liquid Percent composition >98%
Reliability	:	(1) valid without restriction 1d: Meets generally accepted scientific standards and is described in sufficient detail. Klimish rating. Klimish HJ et al, Regulatory Toxicology and Pharmacology 1997; 25:1-5.

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Species	:	rabbit
Concentration	:	undiluted
Dose	:	.5 ml
Exposure time	:	
Comment	:	
Number of animals	:	4
Vehicle	:	none
Result	:	
Classification	:	
Method	:	other:method not indicated
Year	:	
GLP	:	no data

Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Method not indicated, however, the method may have followed that described in the article by Carpenter and Smyth, "Chemical Burns of the Rabbit Cornea", American Journal of Opthalmology, 1947.
Result	:	Four rabbit eyes were apparently unharmed and a fifth suffered only trace injuries following the instillation of an excess (0.5 ml) of the undiluted chemical. Grade 1 in a 10 grade rating system. There were no corneal injuries.
Reliability	:	(3) invalid 3b; Invalid Significant metholodological deficiencies. Klimish rating. Klimish HJ et al, Regulatory Toxicology and Pharmacology 1997; 25:1-5. This study is considered invalid because as per the OECD guideline 0.1 ml is stated amount of test material to instill into the eye. This study instilled 0.5 ml.

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5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT